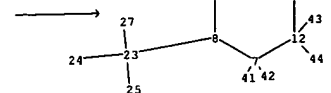
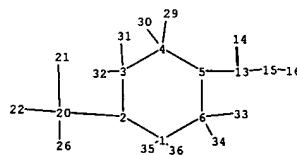
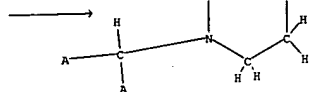
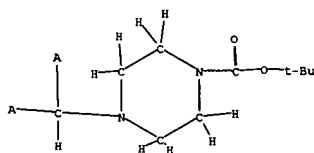


CAS React

NP



chain nodes :

13 14 15 16 17 20 23 26 27 29 30 31 32 33 34 35 36 37 38 39 40 41
42 43 44

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring/chain nodes :

21 22 24 25

chain bonds :

1-35 1-36 2-20 3-31 3-32 4-29 4-30 5-13 6-33 6-34 7-41 7-42 8-23 9-39 9-40
10-37 10-38 11-17 12-43 12-44 13-14 13-15 15-16 20-21 20-22 20-26 23-24 23-25
23-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

1-2 1-6 2-3 2-20 3-4 4-5 5-6 5-13 7-8 7-12 8-9 8-23 9-10 10-11 11-12 13-14
13-15 20-21 20-22 23-24 23-25

exact bonds :

1-35 1-36 3-31 3-32 4-29 4-30 6-33 6-34 7-41 7-42 9-39 9-40 10-37 10-38
11-17 12-43 12-44 15-16 20-26 23-27

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS
33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS
42:CLASS 43:CLASS 44:CLASS

fragments assigned product role:

containing 7

fragments assigned reactant/reagent role:

containing 1

10/076448

=>

Uploading 10076448.str

L3 STRUCTURE UPLOADED

=> s l3

SAMPLE SEARCH INITIATED 18:16:31 FILE 'CASREACT'

SCREENING COMPLETE - 93 REACTIONS TO VERIFY FROM 10 DOCUMENTS

100.0% DONE 93 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 1282 TO 2438
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3 (0 REACTIONS)

=> s l3 sss full

FULL SEARCH INITIATED 18:16:39 FILE 'CASREACT'

SCREENING COMPLETE - 2203 REACTIONS TO VERIFY FROM 180 DOCUMENTS

100.0% DONE 2203 VERIFIED 26 HIT RXNS 2 DOCS
SEARCH TIME: 00.00.01

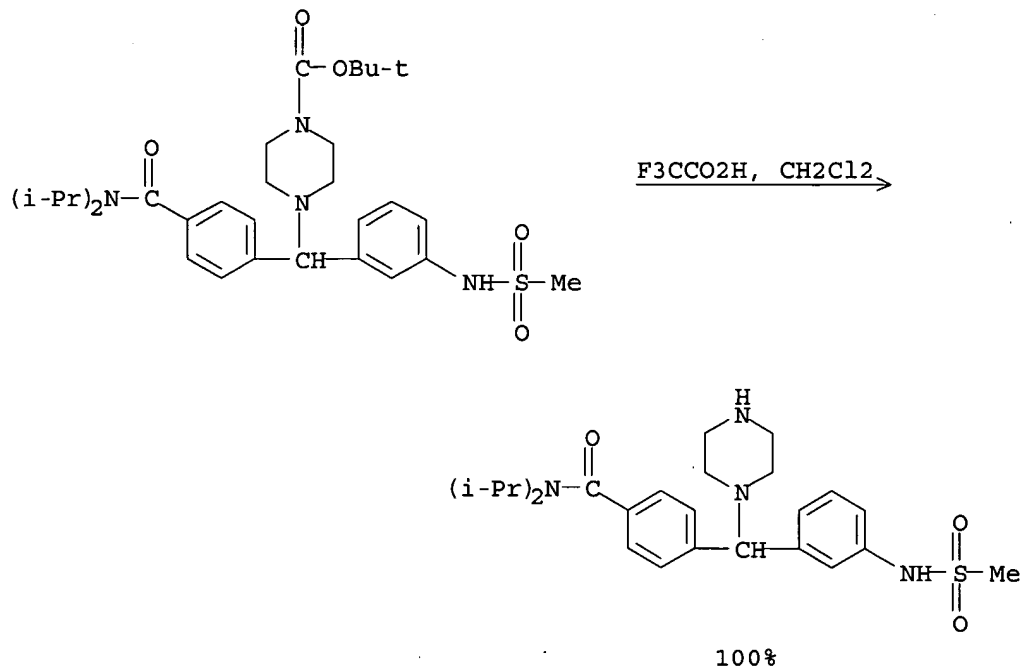
L5 2 SEA SSS FUL L3 (26 REACTIONS)

=> d 1-2 crd

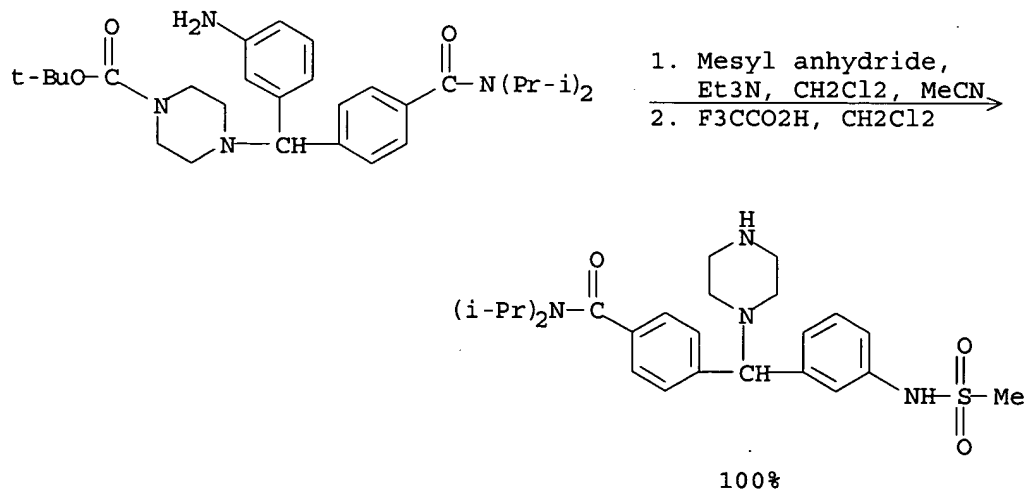
10/076448

L5 ANSWER 1 OF 2 CASREACT COPYRIGHT 2003 ACS

RX(18) OF 48

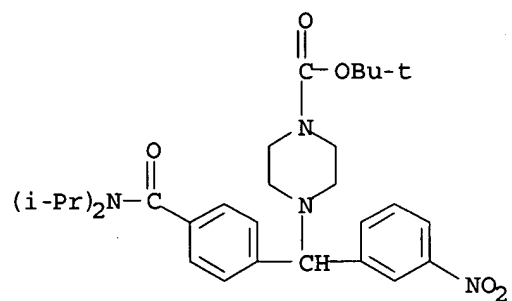


RX(37) OF 48 - 2 STEPS

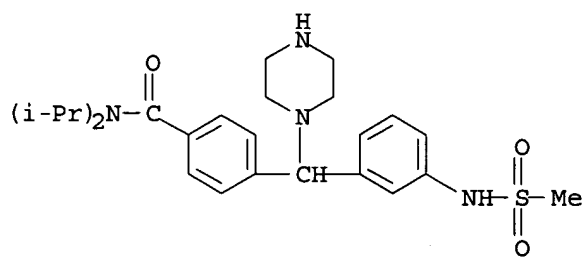


10/076448

RX(44) OF 48 - 3 STEPS



1. Pd, H₂, AcOH
2. Mesyl anhydride,
Et₃N, CH₂Cl₂, MeCN
3. F₃CCO₂H, CH₂Cl₂

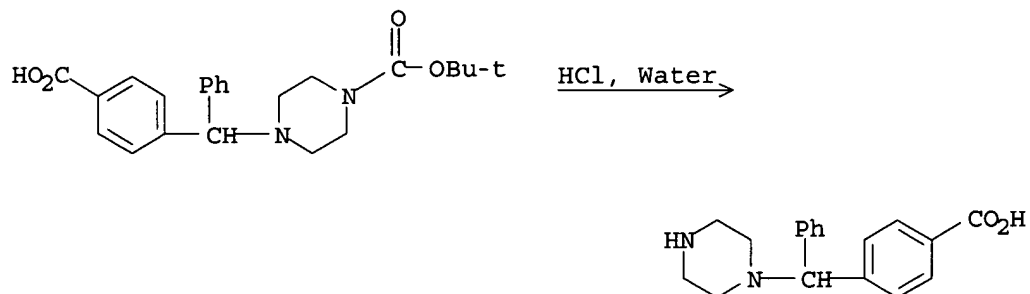


100%

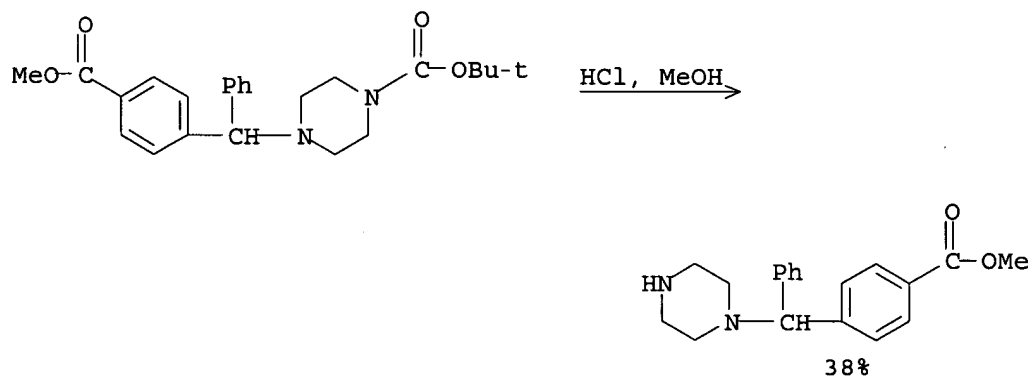
10/076448

L5 ANSWER 2 OF 2 CASREACT COPYRIGHT 2003 ACS

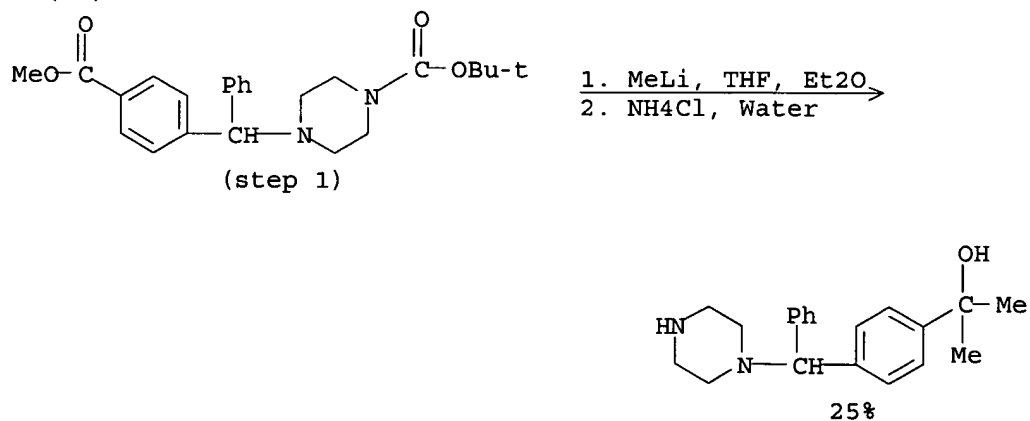
RX(19) OF 401



RX(22) OF 401

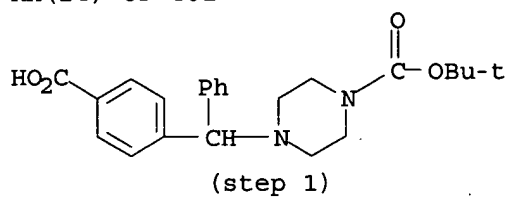


RX(23) OF 401

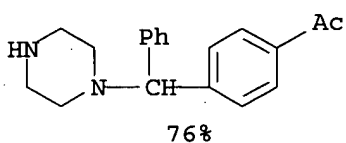


10/076448

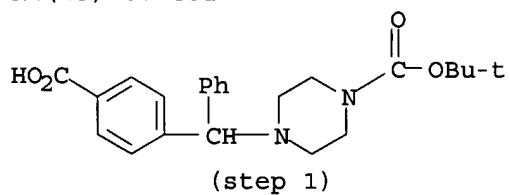
RX(24) OF 401



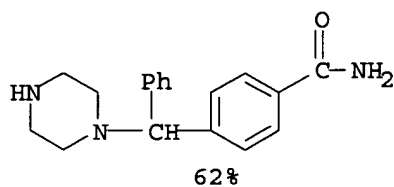
1. MeLi, THF, Et₂O
2. Me₃SiCl
3. NH₄Cl, Water



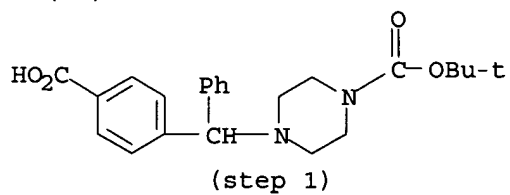
RX(25) OF 401



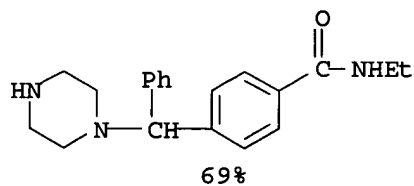
1. Et₃N, ClCO₂Bu-i, THF
2. NH₃, CH₂Cl₂
3. F₃CCO₂H, CH₂Cl₂



RX(26) OF 401

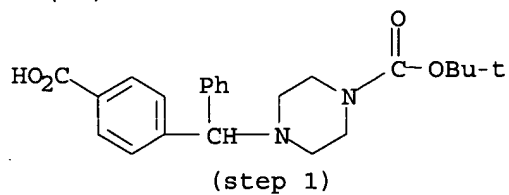


1. Et₃N, ClCO₂Bu-i, THF
2. EtNH₂
3. F₃CCO₂H, CH₂Cl₂

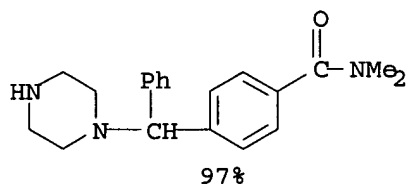


10/076448

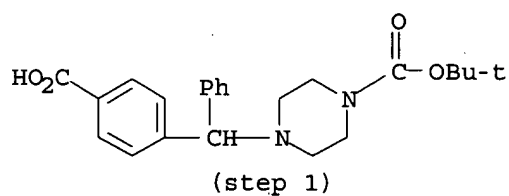
RX(27) OF 401



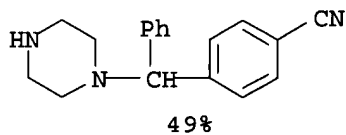
1. Et₃N, ClCO₂Bu-i, THF
2. Me₂NH, THF
3. F₃CCO₂H, CH₂Cl₂



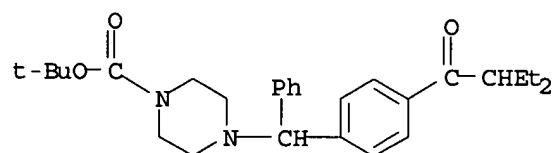
RX(28) OF 401



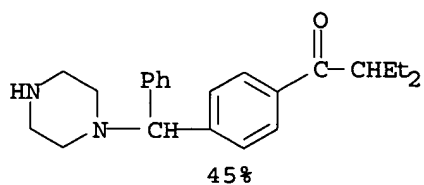
1. Et₃N, ClCO₂Bu-i, THF
2. NH₃, CH₂Cl₂
3. Pyridine, (CF₃CO)₂O, THF
4. HCl, MeOH



RX(39) OF 401

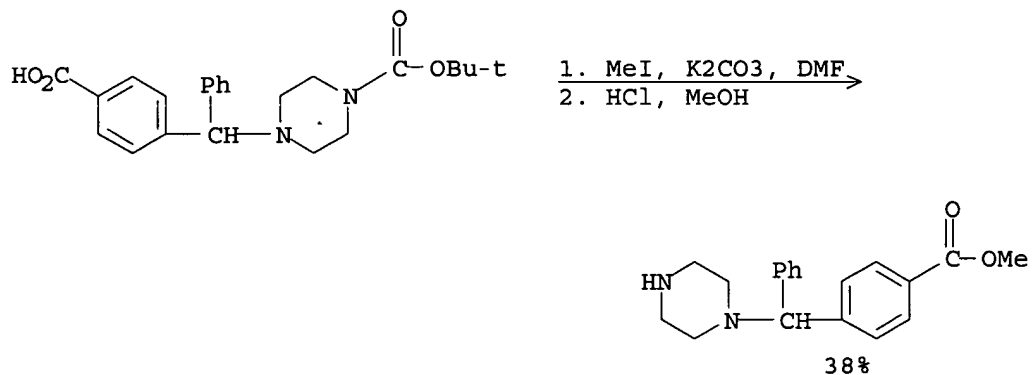


HCl, AcOH, Water

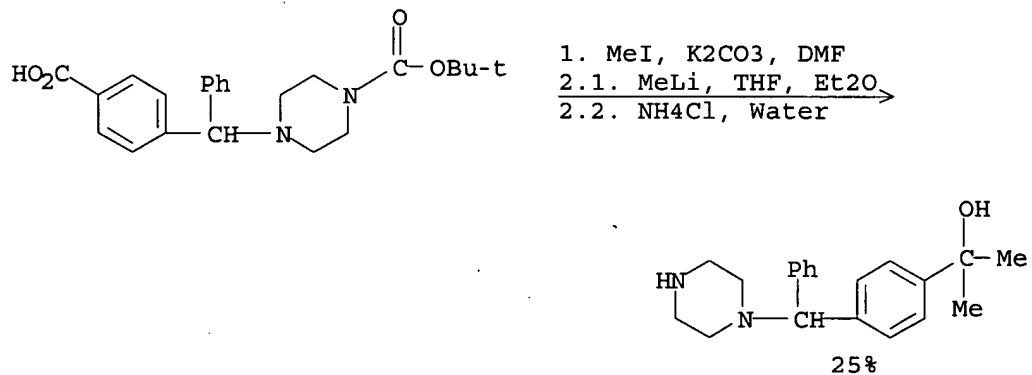


10/076448

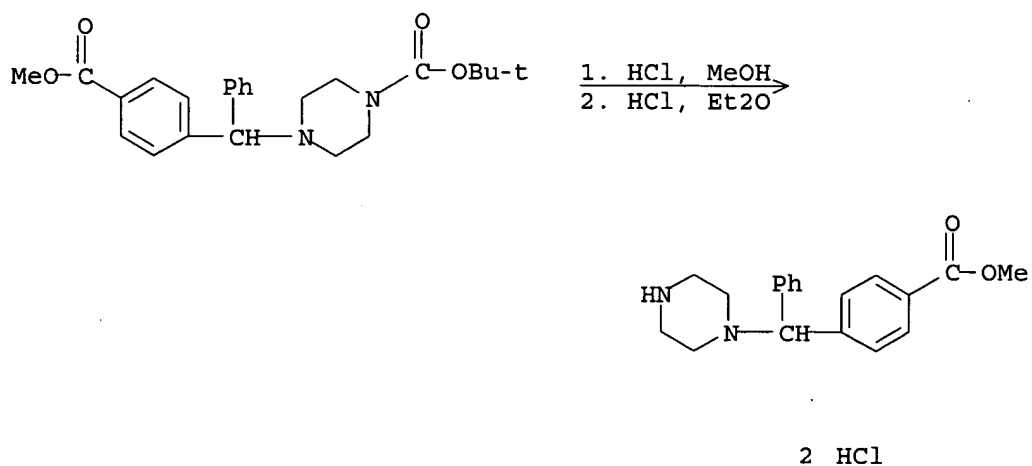
RX(148) OF 401 - 2 STEPS



RX(149) OF 401 - 2 STEPS

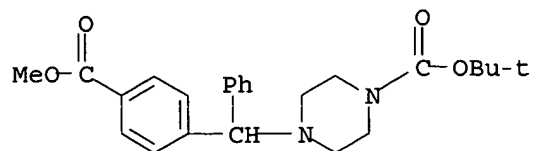


RX(150) OF 401 - 2 STEPS

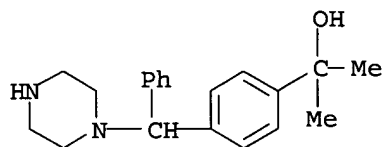


10/076448

RX(151) OF 401 - 2 STEPS

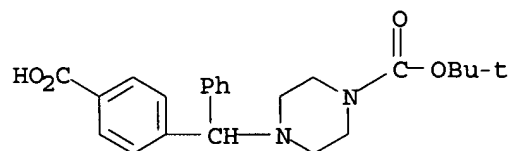


1.1. MeLi, THF, Et2O
1.2. NH4Cl, Water
2. HCl, Et2O

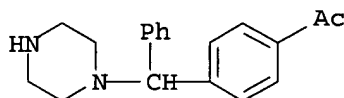


2 HCl

RX(152) OF 401 - 2 STEPS



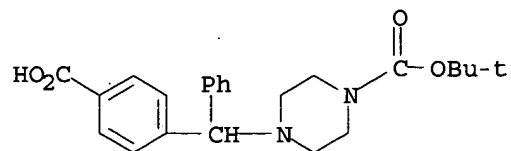
1.1. MeLi, THF, Et2O
1.2. Me3SiCl
1.3. NH4Cl, Water
2. HCl, Et2O



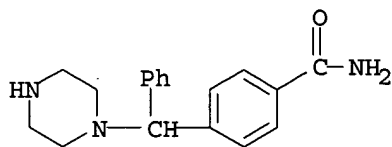
2 HCl

10/076448

RX(153) OF 401 - 2 STEPS

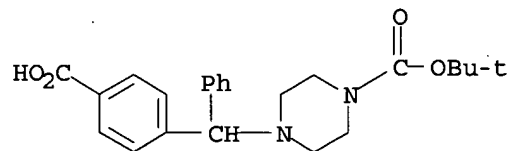


- 1.1. Et_3N , $\text{ClCO}_2\text{Bu-i}$, THF
- 1.2. NH_3 , CH_2Cl_2
- 1.3. $\text{F}_3\text{CCO}_2\text{H}$, CH_2Cl_2
2. HCl , Et_2O

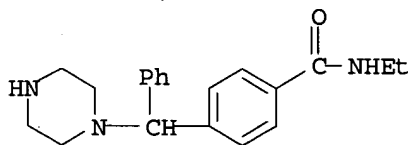


2 HCl

RX(154) OF 401 - 2 STEPS



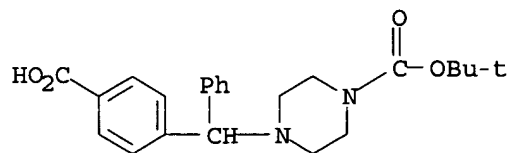
- 1.1. Et_3N , $\text{ClCO}_2\text{Bu-i}$, THF
- 1.2. EtNH_2
- 1.3. $\text{F}_3\text{CCO}_2\text{H}$, CH_2Cl_2
2. HCl , Et_2O



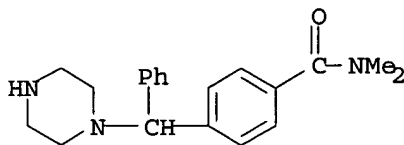
2 HCl

10/076448

RX(155) OF 401 - 2 STEPS

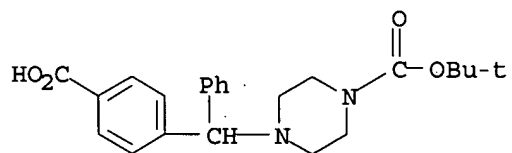


- 1.1. Et₃N, ClCO₂Bu-i, THF
- 1.2. Me₂NH, THF
- 1.3. F₃CCO₂H, CH₂Cl₂
2. HCl, Et₂O

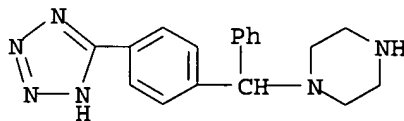


2 HCl

RX(156) OF 401 - 2 STEPS



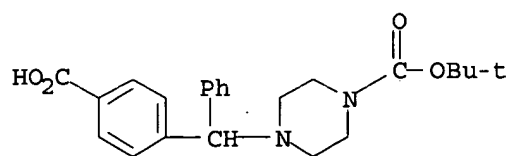
- 1.1. Et₃N, ClCO₂Bu-i, THF
- 1.2. NH₃, CH₂Cl₂
- 1.3. Pyridine, (CF₃CO)₂O, THF
- 1.4. HCl, MeOH
- 2.1. R:1118-03-2, PhMe
- 2.2. R:1118-03-2
- 2.3. HCl, MeOH



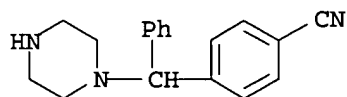
22%

10/076448

RX(157) OF 401 - 2 STEPS

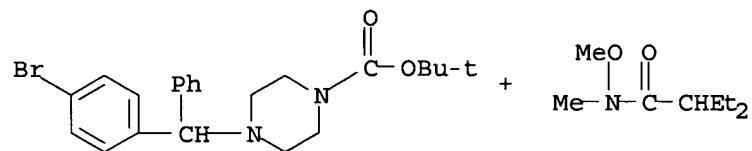


- 1.1. Et3N, ClCO2Bu-i, THF
- 1.2. NH3, CH2Cl2
- 1.3. Pyridine, (CF3CO)2O, THF
- 1.4. HCl, MeOH
2. HCl, Et2O, MeOH

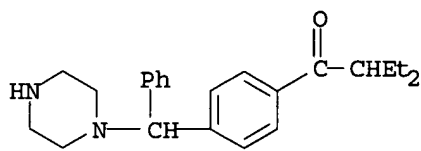


2 HCl

RX(166) OF 401 - 2 STEPS



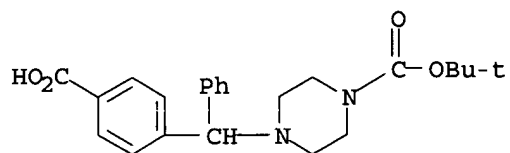
- 1.1. BuLi, THF, Hexane
- 1.2. THF
- 1.3. NH4Cl, Water
2. HCl, AcOH, Water



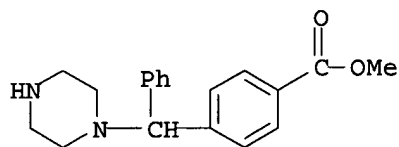
45%

10/076448

RX(294) OF 401 - 3 STEPS

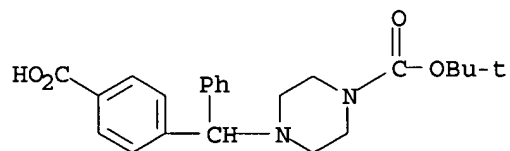


1. MeI, K₂CO₃, DMF
2. HCl, MeOH
3. HCl, Et₂O

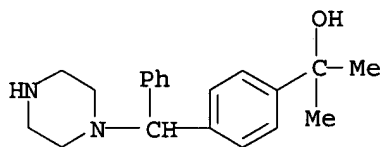


2 HCl

RX(295) OF 401 - 3 STEPS



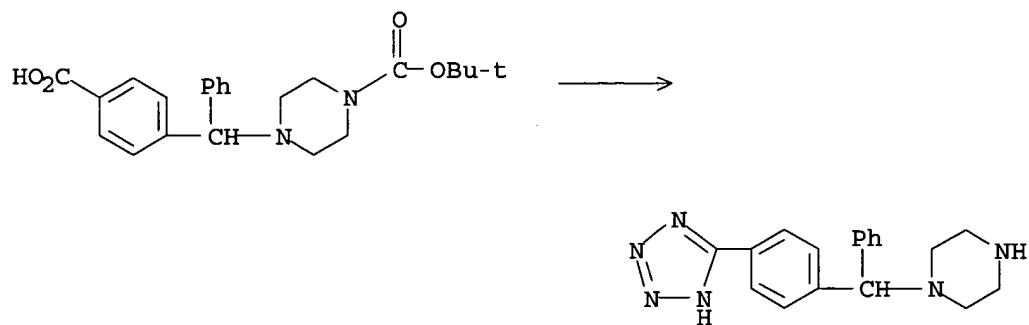
1. MeI, K₂CO₃, DMF
- 2.1. MeLi, THF, Et₂O
- 2.2. NH₄Cl, Water
3. HCl, Et₂O



2 HCl

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RX(298) OF 401 - 3 STEPS



2 HCl

10/076448

=> d 1-2 bib

10/076448

L5 ANSWER 1 OF 2 CASREACT COPYRIGHT 2003 ACS
AN 138:4616 CASREACT
TI Preparation of 4-(phenyl-piperazinyl-methyl)-benzamides as .delta. opioid
receptor agonists for the treatment of pain, anxiety or gastrointestinal
disorders
IN Brown, William; Walpole, Christopher; Plobeck, Niklas
PA Astrazeneca Ab, Swed.
SO PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002094794	A1	20021128	WO 2002-SE956	20020516
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRAI	SE 2001-1772		20010518		
	SE 2001-3820		20011115		

OS MARPAT 138:4616

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/076448

L5 ANSWER 2 OF 2 CASREACT COPYRIGHT 2003 ACS
AN 134:4912 CASREACT
TI New Diarylmethylpiperazines as Potent and Selective Nonpeptidic .delta.
Opioid Receptor Agonists with Increased In Vitro Metabolic Stability
AU Plobeck, Niklas; Delorme, Daniel; Wei, Zhong-Yong; Yang, Hua; Zhou, Fei;
Schwarz, Peter; Gawell, Lars; Gagnon, Helene; Pelcman, Benjamin; Schmidt,
Ralf; Yue, Shi Yi; Walpole, Christopher; Brown, William; Zhou, Edward;
Labarre, Maryse; Payza, Kemal; St-Onge, Stephane; Kamassah, Augustus;
Morin, Pierre-Emmanuel; Projean, Denis; Ducharme, Julie; Roberts, Edward
CS Departments of Chemistry and Pharmacology, Astra Zeneca R&D Montreal,
Saint-Laurent, QC, H4S 1Z9, Can.
SO Journal of Medicinal Chemistry (2000), 43(21), 3878-3894
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/076448

=> log h

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

111.68

111.89

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 18:18:41 ON 17 JUL 2003